

The Kondo effect in the presence of Van Hove singularities: A numerical renormalization group study

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A numerical renormalization group (NRG) investigation of the one-centre $t - t'$ Kondo problem is performed for the square lattice with account of logarithmic Van Hove singularities (VHS) in the electron density of states. The magnetic susceptibility, entropy and specific heat are calculated. The temperature dependences of the thermodynamic properties in the presence of VHS turn out to be non-trivial. For finite t' inverse logarithm of the corresponding Kondo temperature T_K demonstrates a crossover from the square-root to standard linear dependence on the $s - d$ exchange coupling. The low-temperature behavior of magnetic susceptibility and linear specific heat are investigated, and the Wilson ratio is obtained. For $t' \rightarrow 0$ the Fermi-liquid behavior is broken.

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I. INTRODUCTION

The Kondo effect is extensively studied starting from pioneering works by Kondo [1] who explained the minimum of resistance in metallic alloys owing to resonance $s - d$ scattering of conduction electrons by magnetic impurities. The solution of the Kondo problem [2–4] is a very beautiful chapter in the history of modern theoretical physics.

The Kondo phenomenon is a key for explaining the behavior of heavy-fermion compounds and Kondo lattices [5, 6], non-Fermi-liquid (NFL) systems [7, 8], anomalous electronic properties of metallic glasses [9], quantum dots [10], and other systems. The Kondo anomalies are also studied in systems of reduced dimensionality where they have a number of experimental peculiarities [11]. It is evident that the Kondo effect in such systems has a number of peculiar features from the theoretical point of view too.

The Kondo effect owing to Cu^{2+} spins in the CuO_2 planes is observed in layered n-type cuprates $(\text{La,Ce})_2\text{CuO}_4$, $(\text{Pr,Ce})_2\text{CuO}_4$, and $(\text{Nd,Ce})_2\text{CuO}_{4-\delta}$ [12].

Last time, the Kondo effect in graphene (truly two-dimensional system with a peculiar electron spectrum) is discussed [13–15]. Because of the pseudogap in the spectrum, the Kondo effect for the undoped graphene exists under restricted conditions only, but for a doped substance the Kondo phase is present for all parameters [14].

We can mention also some layered f -systems where experimental investigations and first-principle band calculations demonstrate existence of two-dimensional features in electron properties. Here belong the compounds CeCoIn_5 (where the layers CeIn are present) [16], CeCoGe_2 [17], CePt_2In_7 [18], CeRhIn_5 , Ce_2RhIn_8 [19], $\text{UCo}_{0.5}\text{Sb}_2$ (where two-dimensional weak localization is observed) [20].

The layered Kondo lattice model was proposed for quantum critical beta- YbAlB_4 where two-dimensional boron layers are Kondo coupled via interlayer Yb moments [21]. CeRuPO seems to be one of the rare examples of a ferromagnetic Kondo lattice where LSDA+U calculations evidence a quasi-two-dimensional electronic band structure, reflecting a strong covalent bonding within the CeO and RuP layers and a weak ioniclike bonding between the layers [22].

The above f -systems demonstrate often both local-moment and itinerant-electron features. Large linear specific heat and NFL behavior is observed also in some d -systems including layered ruthenates Sr_2RuO_4 [23] and $\text{Sr}_3\text{Ru}_2\text{O}_7$ [24]. Besides correlation effects, anomalies of electron properties in such systems are owing to the presence of Van Hove singularities near the Fermi level.

In the present work we treat the one-centre Kondo problem with the singular electron density of states. Earlier this problem was considered by Gogolin [25] who used a “fast parquet” approach. In fact, such complicated methods are somewhat ambiguous, and the numerical renormalization group (NRG) results of paper [26] do not agree with the results of Ref.[25]. Therefore we start in Sect. 2 from the standard perturbation theory and also apply the “poor man scaling” approach by Anderson [27].

In Sect. 3 we apply to the problem the NRG method, the technical details for our case being considered in Appendix. The simple perturbation results for the Kondo temperature agree with NRG much better than the parquet results

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[25]. The physical quantities in the presence of the logarithmic singularity near the Fermi level are investigated. We calculate the magnetic susceptibility and specific heat, in particular at low temperatures, discuss the problem if universal behavior and calculate the Wilson ratio.

II. THE KONDO MODEL WITH VAN HOVE SINGULARITIES

We use the Hamiltonian of the one-centre $s - d(f)$ exchange (Kondo) model

$$H_{sd} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} - \sum_{\mathbf{k}\mathbf{k}'\alpha\beta} J_{\mathbf{k}\mathbf{k}'} \mathbf{S} \sigma_{\alpha\beta} c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{k}'\beta} \quad (1)$$

where $\varepsilon_{\mathbf{k}}$ is the band energy, \mathbf{S} are spin operators, σ are the Pauli matrices, in the case of contact coupling $J_{\mathbf{k}\mathbf{k}'} = J/N_s$ where J is the $s - d(f)$ exchange parameter, N_s is the number of lattice sites.

Kondo [1] found that high-order perturbation contributions to various physical properties contain logarithmically divergent corrections. As demonstrated further investigations of the Kondo problem, there occurs a pole at the boundary of strong coupling region, which is called the Kondo temperature (in fact, this is a crossover scale). For a smooth density of states $\rho(E)$ this quantity is estimated as

$$T_K \propto D \exp \frac{1}{2J\rho(0)}, \quad (2)$$

where D is the half-bandwidth. We treat the case of logarithmically divergent bare density of electron states

$$\rho(E) = A \ln \frac{D}{B|E + \Delta|}$$

(the energy is referred to the Fermi level, the constants A , B and Δ are determined by the band spectrum). The logarithmic divergence in $\rho(E)$ is typical for the two-dimensional case (in particular, for the layered ruthenates). However, similar strong Van Hove singularities can occur also in some three-dimensional systems like Pd alloys and weak itinerant ferromagnets ZrZn_2 and TiBr_2 [28, 29].

First we consider perturbation expansion for the resistivity, following to the original approach by Kondo [1]. We write down the inverse transport relaxation time with the Kondo correction

$$\tau^{-1}(E) = \tau_0^{-1}(E)[1 + 4Jg(E, 0)]. \quad (3)$$

Here

$$g(E, T) = \sum_{\mathbf{k}} \frac{1/2 - n_{\mathbf{k}}}{E - \varepsilon_{\mathbf{k}}} = \int dE' \rho(E') \frac{1/2 - f(E')}{E - E'} \quad (4)$$

with $n_{\mathbf{k}} = f(\varepsilon_{\mathbf{k}})$ is the Fermi function. After integration by part, in the case $\Delta = 0$ we obtain to logarithmic accuracy for the resistivity

$$R_{sd} \sim \int dE \rho(E) \left(-\frac{\partial f(E)}{\partial E} \right) \tau_0^{-1}(E) \left[1 - 2AJ \int dE' \left(-\frac{\partial f(E')}{\partial E'} \right) \ln^2 \left| \frac{D}{E'} \right| \right] \quad (5)$$

so that

$$R_{sd} = R_{sd}^{(0)} \left(1 - 2AJ \ln^2 \frac{D}{T} \right), \quad R_{sd}^{(0)} \sim J^2 S(S+1) A \ln \frac{D}{T} \quad (6)$$

Applying the Abrikosov–Suhl summation (see [1]) we get

$$R_{sd} = R_{sd}^{(0)} \left(1 + JA \ln^2 \frac{D}{T} \right)^{-2} \quad (7)$$

which yields a non-standard expression for the Kondo temperature,

$$T_K \simeq D \exp \left[- \left| \frac{1}{AJ} \right|^{1/2} \right]. \quad (8)$$

We calculate also the Kondo corrections to the static impurity magnetic susceptibility by generalizing consideration of Ref.[1] to the case of singular density of states. Expanding to second order in J we derive (cf. [1, 4, 30])

$$\chi(T) = \frac{S(S+1)}{3T} \left[1 + 2J\chi^{(0)} - 2J^2 \sum_{\mathbf{k}\mathbf{k}'} \frac{n_{\mathbf{k}}(1-n_{\mathbf{k}'})}{(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'})^2} \right] \quad (9)$$

where

$$\chi^{(0)}(T) = - \sum_{\mathbf{k}} \frac{\partial n_{\mathbf{k}}}{\partial \varepsilon_{\mathbf{k}}} = \int dE \rho(E) \left(- \frac{\partial f(E)}{\partial E} \right) \simeq A \ln \frac{D}{\max(\Delta - T, T)} \quad (10)$$

is the Pauli susceptibility of non-interacting conduction electrons with the singular density of states, which is shown in Fig.1. For $\Delta \neq 0$ this quantity has a maximum at $T \simeq \Delta/2$. Such a behavior is typical for the case where a density-of-states peak is present near the Fermi level [31].

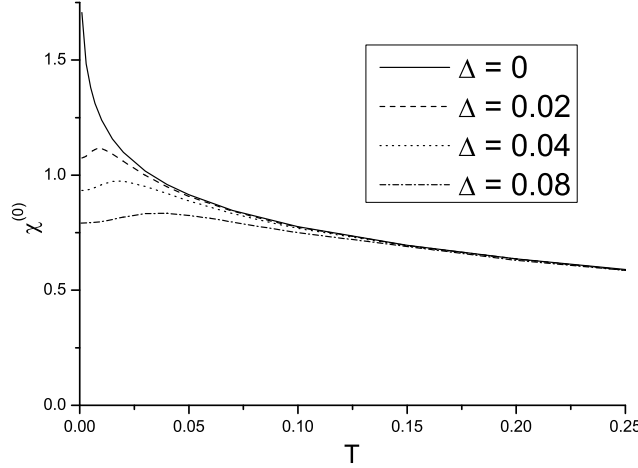


FIG. 1: The temperature dependence of non-interacting magnetic susceptibility for conduction electrons $\chi^{(0)}(T)$ at $\Delta = 0, 0.02, 0.04, 0.08$

Performing integration and summation of the series of logarithmic terms we have

$$\chi(T) = \frac{S(S+1)}{3T} \left[1 + \frac{2J\chi^{(0)}}{1 + J\chi^{(0)} \ln(D/T)} \right] \quad (11)$$

which yields at $\Delta = 0$ the same result for the Kondo temperature (8)

The correction to magnetic impurity entropy can be written down in an analogous way to obtain [1, 4]

$$\mathcal{S}_{\text{imp}}(T) = \ln(2S+1) + \frac{\pi^2}{3} \frac{S(S+1)}{[1 + J\chi^{(0)} \ln(D/T)]^3} [2J\chi^{(0)}]^3 \quad (12)$$

Then we have for impurity specific heat

$$C_{\text{imp}}(T) = T \frac{d\mathcal{S}_{\text{imp}}(T)}{dT} = \frac{\pi^2 S(S+1)}{[1 + J\chi^{(0)} \ln(D/T)]^4} \left([2J\chi^{(0)}]^4 + 8J^3 T \frac{d\chi^{(0)}}{dT} [\chi^{(0)}]^2 \right) \quad (13)$$

The first term in the brackets yields the same structure as in the case of a smooth density of states (where $\chi^{(0)} = \rho$ and the singular contribution occurs in the fifth order in J only), and the second term is owing to logarithmic singularity in $\chi^{(0)}$. Being of the third order in J , the latter term can dominate. Beside that, it can change its sign and become negative; as we shall see below in Sect.3, this is important for the $C_{\text{imp}}(T)$ behavior.

Of course, the above expressions are applicable for $T > T_K$ only.

To perform a more formal consideration, we can apply the “poor man scaling” approach [27]. This treats the dependence of effective (renormalized) model parameters on the cutoff parameter C which occurs at picking out

the singular contributions from the Kondo corrections to the effective coupling $J_{ef}(C)$ (with $J_{ef}(-D) = J$). The second-order singular correction to $J_{ef}(C)$ can be obtained in the form [32]

$$\delta J_{ef} = -2J^2 \sum_{\mathbf{k}} \frac{n_{\mathbf{k}}}{E - \varepsilon_{\mathbf{k}}} \quad (14)$$

Picking out in the sum the contribution of intermediate electron states near the Fermi level with $C < \varepsilon_{\mathbf{k}} < C + \delta C$ we obtain

$$\delta J_{ef}(C) = 2AJ^2 \ln \frac{D}{|C + \Delta|} \frac{\delta C}{C} \quad (15)$$

Replacing in the right-hand part $J \rightarrow J_{ef}(C)$ we obtain

$$\frac{\partial}{\partial C} \frac{1}{J_{ef}(C)} = -\frac{2A}{C} \ln \frac{D}{|C + \Delta|} \quad (16)$$

Solving this equation for $T_K \gg \Delta$ we get

$$\frac{1}{J_{ef}(C)} = \frac{1}{J} + A \ln^2 \left| \frac{D}{C} \right|. \quad (17)$$

Then we obtain from the condition $1/J_{ef}(T_K) = 0$ again the result (8).

One can see that the expression (8) is different from the corresponding parquet result [25]

$$T_K \simeq D \exp \left[- \left| \frac{2}{AJ} \right|^{1/2} \right]. \quad (18)$$

However, the NRG calculations [26] confirms the perturbation expression (8) rather than (18) (see the discussion below). The corresponding problems of the parquet approximation in the Hubbard model are discussed in the works [33].

III. RESULTS OF NUMERICAL CALCULATIONS

We consider $S = 1/2$ Kondo model for the square lattice with the spectrum

$$\varepsilon_{\mathbf{k}} = 2t(\cos k_x + \cos k_y) + 4t'(\cos k_x \cos k_y + 1)$$

The corresponding density of states is

$$\rho(E) = \frac{1}{2\pi^2 \sqrt{t^2 + Et' - 4t'^2}} K \left(\sqrt{\frac{t^2 - E^2/16}{t^2 + Et' + 4t'^2}} \right) \simeq \frac{1}{2\pi^2 \sqrt{t^2 - 4t'^2}} \ln \frac{16\sqrt{t^2 - 4t'^2}}{|E + 8t'|} \quad (19)$$

where $K(E)$ is the complete elliptic integral of the first kind. In the numerical calculations, the Fermi level is supposed to be located in the band centre, so that the band is determined by $|E| < D = 4|t|$. The distance from the Van Hove singularity to the Fermi level is $\Delta = 8t'$. When presenting numerical results, we put $D = 1$.

For $t' = 0$ we derive

$$\rho(E) = \frac{2}{\pi^2 D} K \left(\sqrt{1 - \frac{E^2}{D^2}} \right) \simeq \frac{2}{\pi^2 D} \ln \frac{4D}{|E|}, \quad (20)$$

so that, according to (8),

$$T_K \simeq D \exp \left[- \left| \frac{\pi^2 D}{2J} \right|^{1/2} \right]. \quad (21)$$

The details of NRG calculations are discussed in Appendix.

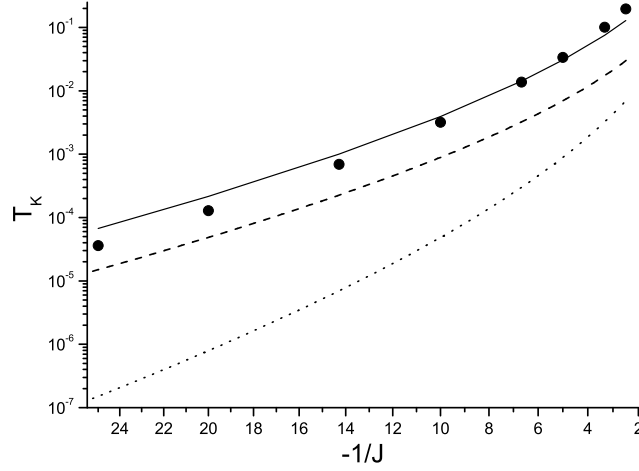


FIG. 2: The dependence $T_K(J)$ for $t' = 0$. Circles are NRG results, solid line corresponds to the Nagaoka-Suhl formula (22), dashed line to Eq.(21) and dotted one to Eq.(18) (without any fitted preexponential constants)

The Kondo temperature in NRG calculations is determined from the temperature dependence of impurity magnetic susceptibility $\chi_{\text{imp}}(T)$ by using condition $T_K \chi_{\text{imp}}(T_K) = 0.0701$ that is standard in the NRG method [2].

Figs.2, 3 show the dependence of the Kondo temperature on the bare coupling $|J|$ in the logarithmic scale. One can see that for finite t' there occurs a crossover with decreasing $|J|$ from the square-root dependence (8) to the standard Kondo behavior (2). This crossover is qualitatively described by the lowest-order scaling.

It should be noted that the Kondo phenomenon should be invariant under particle-hole transformation ($\varepsilon_{\mathbf{k}} \rightarrow -\varepsilon_{\mathbf{k}}$, i.e., $\rho(\epsilon) \rightarrow \rho(-\epsilon)$). However, in the case of a non-symmetric density of states using the formula $1 = 2Jg(T_K, 0)$ (where $g(E, T)$ is determined by (4)) yields slightly different results for the peak above and below the Fermi level. Therefore we use the Nagaoka-Suhl formula (see [1])

$$1 = 2Jg(0, T_K) \quad (22)$$

which works somewhat better at large J , but slightly worse at small J . (In fact, all such approximations yield nearly the same result at small J .)

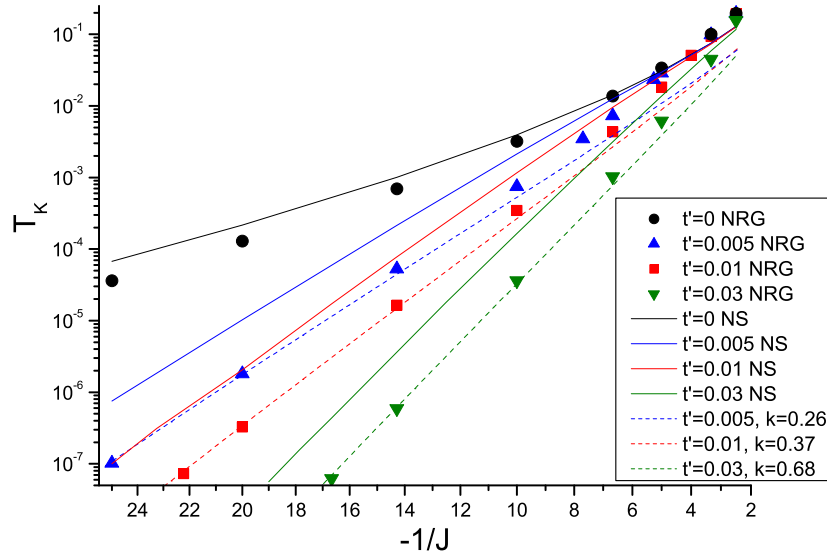


FIG. 3: Fitting of the dependences $T_K(J)$ for $t' = 0, 0.005, 0.01, 0.03$. Circles, top-up triangles, squares and top-down triangles are corresponding NRG results, solid lines (from above to below) correspond to the Nagaoka-Suhl formula (22), dashed lines (from above to below) show the two-loop result (23) with fitted constants k

According to (16), for $\Delta \ll T_K$ we have $\ln T_K \sim 1/\sqrt{|J|}$ and for $\Delta \gg T_K$ we come to the standard linear behavior

$\ln T_K \sim 1/|J|$ with enhanced $\rho(0)$. For intermediate J , a crossover takes place.

The lowest-order scaling describes satisfactorily the numerical data at large $|J|$. However, it is insufficient to fit the numerical results at small $|J|$. Therefore we use the two-loop scaling result [2, 4]

$$T_K = kD|2J\rho|^{1/2} \exp[1/2J\rho] \quad (23)$$

This expression implies that only small vicinity of the Fermi surface with nearly constant $\rho(E) \simeq \rho$ works. This assumption becomes not valid with increasing $|J|$ since the whole logarithmic peak becomes important. It should be noted that, as follows from the structure of scaling equations (see Ref.[4]), the factor of $|2J\rho|^{1/2}$ does not occur in the expression for T_K at $\Delta = 0$.

The fitted constant k should be determined by the whole form of the function $\rho(E)$. At small t' , k is small since the quantity $\rho(0)$ is large owing to peaks. On the contrary, for larger $t' = 0.03 - 0.05$, $\rho(0)$ becomes small.

Since T_K is high in our case of singular density of states, consideration of the situation with $\Delta \sim T_K$ is quite realistic. We can see that appreciable deviations owing to the singularity occur even if Δ is not too small and exceeds T_K .

The magnetic susceptibility owing to impurity can be expressed as a difference of magnetic susceptibilities of the whole system and the system without impurity:

$$\chi(T) \equiv \chi_{\text{imp}}(T) = \chi_{\text{tot}}(T) - \chi_{\text{band}}(T), \quad (24)$$

where χ_{tot} is the total magnetic susceptibility, and $\chi_{\text{band}} = 2N_s\chi^{(0)}$ is the susceptibility of non-interacting band electrons (for two spin projections). Apart from the susceptibility (24), the so-called local magnetic susceptibility χ_{loc} is frequently introduced as well:

$$\chi_{\text{loc}}(T) = \int_0^{1/T} \langle S_z(\tau) S_z \rangle d\tau, \quad (25)$$

This is the susceptibility of a *single* impurity in a magnetic field that acts locally, only on this impurity; its magnitude, therefore, can hardly be measured experimentally, in contrast to χ_{imp} .

In principle, χ_{imp} and χ_{loc} can behave quite differently. This possibility was mentioned in Ref.[34], where the reason for the difference is related to the energy dependence $\rho(E)$ and is asserted that this disappears for a flat band of half-width D in the limit of $D \rightarrow \infty$.

The impurity entropy and specific heat are defined in a similar way.

Figs.4-6 show the temperature dependence of magnetic susceptibility for different t' values. At high temperatures, $\chi(T)$ obeys the Curie law, and at low temperatures it demonstrates the Pauli behavior (except for the case $\Delta \rightarrow 0$).

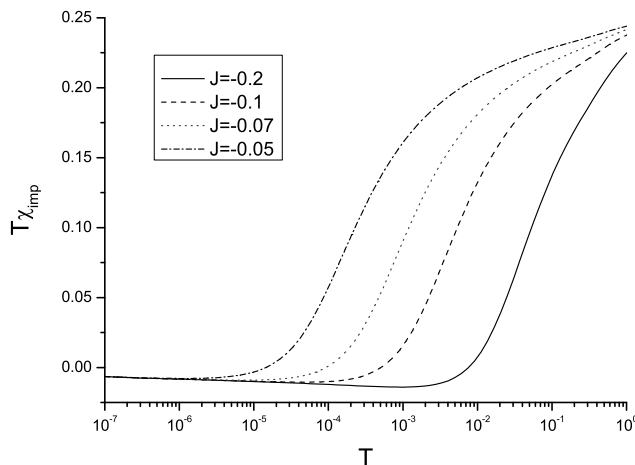


FIG. 4: The temperature dependence $T\chi_{\text{imp}}(T)$ for $t' = 0$ and $J = -0.2, -0.1, -0.07, -0.05$ (lines from below to above)

For the standard flat-band case we have $T\chi(T) = \phi(T/T_K)$, so that the curves $T\chi(T)$ are universal: a change in J results in a change of T_K only. In our situation, such a simple universality does not hold. In particular, for $t' = 0$ this fact (illustrated by Fig.4) was demonstrated in Ref.[26].

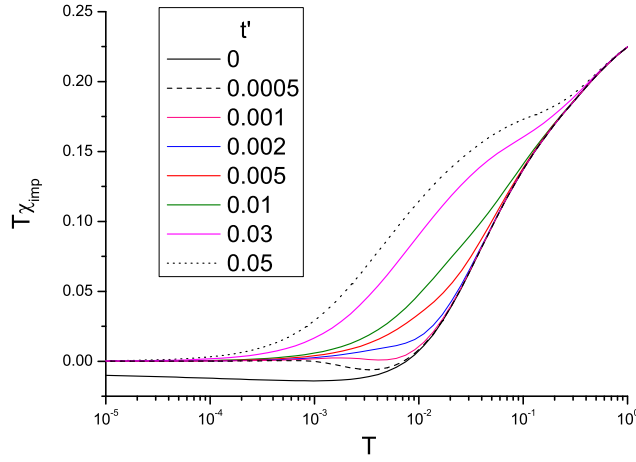


FIG. 5: The temperature dependence $T\chi_{\text{imp}}(T)$ for $J = -0.2$ and different $t' = 0, 0.0005, 0.001, 0.002, 0.005, 0.01, 0.03, 0.05$ (lines from below to above)

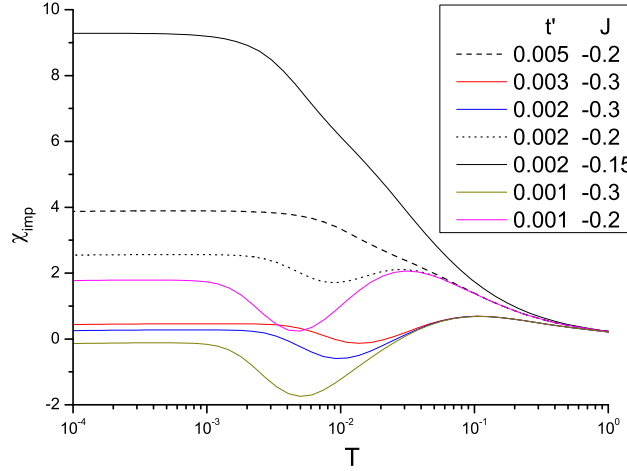


FIG. 6: The temperature dependence $\chi_{\text{imp}}(T)$ for different J and t'

One can see from Fig.6 that the minimum of $\chi(T)$ occurs with decreasing Δ , its position being determined by the maximum of $\chi^{(0)}(T)$ in Eq.(10). This minimum is due to the strong energy dependence of the bare density of states, see Eqs.(9)-(11). Thus, besides the Kondo temperature T_K , a second characteristic scale can occur in our problem, which is determined by Δ . Therefore we have to discuss the meaning of the Kondo temperature T_K in more detail. This quantity comes from the expansion in J starting from high temperatures where impurity susceptibility $\chi(T)$ obeys the Curie law. T_K is determined as a temperature scale where a considerable deviation from this law occurs. In the flat-band situation and for smooth $\rho(E)$, $\chi(T)$ decreases monotonously with increasing T , the universal behavior taking place. This picture is characterized by the ratio $w = 4T_K\chi(0) \approx 0.41$ [2-4] which relates high- and low-temperature scales T_K and $\chi(0)$. Such a behavior holds for $T_K < \Delta$, but for small Δ values the universality is broken, so that the intermediate-temperature dependence $\chi(T)$ becomes complicated and w deviates from 0.41 (see Table I).

The Wilson ratio $R = (4\pi^2/3)\chi_{\text{imp}}(0)/\gamma_{\text{imp}}$ relating low-temperature susceptibility and linear specific heat γ_{imp} is also presented in the Table I. It is important that even for rather small Δ the value of R is still close to 2. Therefore a Fermi-liquid behavior, characteristic for the Kondo problem [2], is restored at low temperatures, except for the case of extremely small Δ where $\chi_{\text{imp}}(0)$ and $C_{\text{imp}}(0)$ can even become negative.

Occurrence of negative values of χ_{imp} and \mathcal{S}_{imp} was demonstrated in Ref.[26] by a strict analytical consideration of the simple case $J = -\infty$ for the semielliptic density of states. This is a common property of systems with very narrow density of states peaks near the Fermi level. Of course, the quantities χ_{tot} and χ_{band} remain positive.

In the standard situation of Kondo effect one has $T\chi(T) = O(T)$, so that the impurity moment (note that $T\chi = \langle S_z^2 \rangle_{\text{tot}} - \langle S_z^2 \rangle_{\text{band}}$, see Appendix) is completely compensated by conduction electrons. At the same time, in the

TABLE I: Results of our NRG calculations for different t' and J : T_K (first line); Wilson ratio R (second line); the quantity $w = 4T_K\chi(0)$ (third line; Wilson's value is $w = 0.4128 \pm 0.002$)

t'	$J = -0.1$	$J = -0.15$	$J = -0.2$	$J = -0.3$
0.05	$1.19 \cdot 10^{-5}$	$4.76 \cdot 10^{-4}$	0.00333	0.0277
	2.008	2.008	2.014	1.99
	0.414	0.416	0.416	0.415
0.03	$3.62 \cdot 10^{-5}$	0.00103	0.00613	0.0450
	1.995	1.988	2.005	1.98
	0.413	0.413	0.414	0.413
0.01	$3.45 \cdot 10^{-4}$	0.00436	0.0184	0.0930
	1.998	1.995	1.991	2.12
	0.415	0.416	0.425	0.386
0.005	$7.49 \cdot 10^{-4}$	0.00726	0.0288	0.0989
	1.999	1.997	2.069	2.237
	0.416	0.418	0.447	0.268736
0.003	0.00112	0.0102	0.0320	0.100007
	2.002	1.992	1.998	3.18
	0.417	0.449	0.392	0.184
0.002	0.00144	0.0121	0.0330	0.1004
	1.996	1.97	2.040	-177 ^a
	0.417	0.44768	0.337	0.108
0.001	0.00208	0.0134	0.0337	0.1006
	1.989	2.03	2.41	0.343 ^b
	0.43	0.38	0.24	-0.048

^a $\chi(0) = 0.27$, $\gamma_{\text{imp}} = -0.02$

^b $\chi(0) = -0.12$, $\gamma_{\text{imp}} = -4.6$

pseudogap situation (low density of states near E_F , $\rho(E) \propto |E - E_F|^r$, $r > 0$) the screening is incomplete, $T\chi(T) > 0$ [35]. Our problem describes the opposite situation: $\rho(E \rightarrow 0)$ diverges and we have overcompensation: $T\chi(T) < 0$.

The singular case $\Delta \rightarrow 0$ demonstrates essentially non-Fermi-liquid behavior (divergence of impurity magnetic susceptibility and specific heat at $T \rightarrow 0$). This situation of singular density of states at the Fermi level is somewhat similar to the overscreened Kondo problem [36] where the number of scattering channel of conduction electrons $n > 2S$ (S is the localized spin value); in this case $\chi(T)$ demonstrates power-law behavior, but remains positive. The low-temperature behavior at $\Delta = 0$ can be fit as [26]

$$\chi_{\text{imp}} = -\frac{A}{T|\ln(T/D)|^\alpha}, A \approx 0.072, \alpha \approx 0.77 \quad (26)$$

$$\mathcal{S}_{\text{imp}} = -\frac{B}{|\ln(T/D)|^\delta}, B \approx 1.065, \delta \approx 0.89. \quad (27)$$

(see Fig.7), so that

$$C_{\text{imp}} = -\frac{B\delta}{|\ln(T/D)|^{\delta+1}}. \quad (28)$$

These asymptotics are independent of J (cf. Fig.4) since at sufficiently low temperatures any value of $|J|$ manifold exceeds both the temperature and the width of the infinitely thin logarithmic peak in $\rho(E)$.

According to Ref.[37], the NFL behavior with $C \propto 1/\ln^4(T_K/T)$ takes place in the case of underscreened ($S > 1/2$) Kondo problem [37].

Fig. 8 shows the temperature dependence of impurity specific heat $C_{\text{imp}} = C_{\text{tot}} - C_{\text{band}}$ for different t' . As a rule, this dependence demonstrates two peaks. At not too small Δ , the high-temperature maximum occurs at the temperature, determined by the distance from VHS to E_F . This is owing to the non-monotonous dependence of $\chi^{(0)}(T)$, see Eqs.(10), (13). When decreasing temperature and passing this maximum, $C_{\text{imp}}(T)$ acquires a minimum and even can become negative. The low-temperature peak is owing to the Kondo effect and takes place in the standard flat-band situation too (see Ref. [39]). One can see that its position corresponds roughly to the Kondo temperature. For small $\Delta < T_K$, the order of positions of the maxima becomes interchanged.

The corresponding magnetic entropy \mathcal{S}_{imp} is shown in Fig. 9. One can see that this quantity tends to the value $\ln 2 = \ln(2S + 1)$ at high temperatures and demonstrates the Kondo compensation at low temperatures. The behavior turns out to be non-monotonous due to the maximum in $\chi^{(0)}(T)$ (see Eq.(12)).

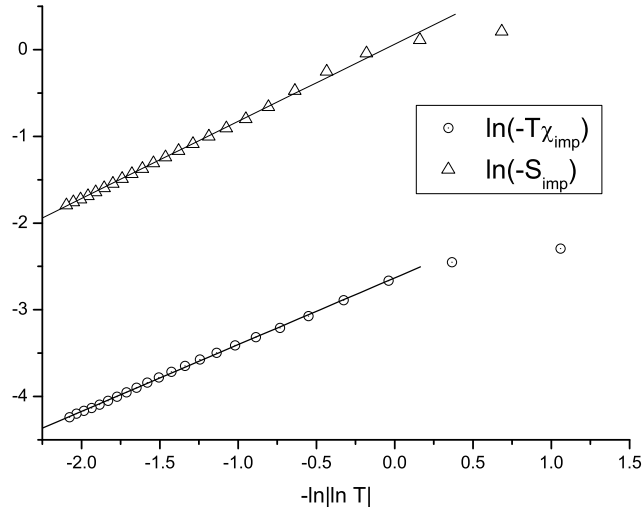


FIG. 7: The fitting of thermodynamic properties at low temperatures for $\Delta = 0$

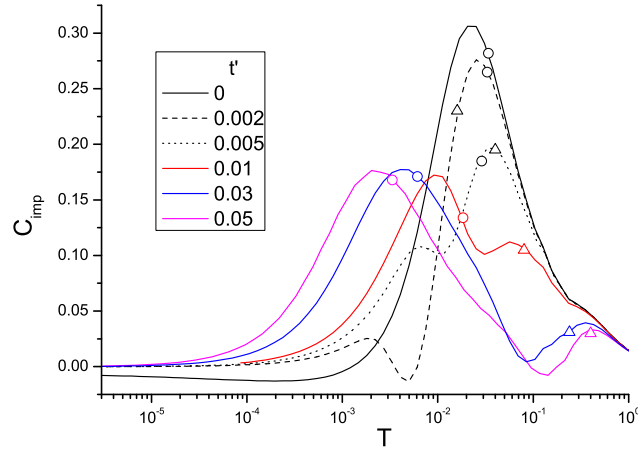


FIG. 8: The temperature dependence of impurity specific heat for $J = -0.2$ and different $t' = 0, 0.002, 0.005, 0.01, 0.03, 0.05$ (lines from below to above, if one sees the left-hand part of the figure); circles mark T_K , and triangles Δ

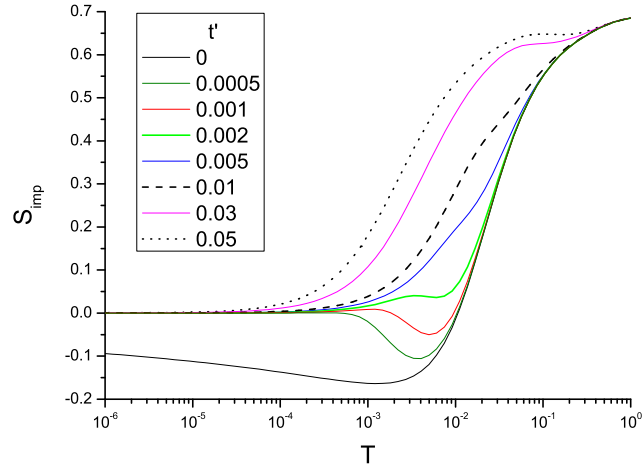


FIG. 9: The temperature dependence of magnetic entropy for $J = -0.2$ and different $t' = 0, 0.0005, 0.001, 0.002, 0.005, 0.01, 0.03, 0.05$ (lines from below to above)

IV. CONCLUSIONS

In the general problem of magnetism of metals and alloys, the peaks in the bare density of states (which are usually owing to Van Hove singularities) near the Fermi level play a crucial role. The correlation effects can result in a considerable qualitative and quantitative modification of the corresponding temperature dependences [28]. They can be important, e.g., for transition-metal alloys.

The considered $t - t'$ Kondo problem which includes VHS is a non-trivial example of influence of density-of-states peaks on electron properties being combined with correlation effects [28, 31]. Our treatment gives an example of exact numerical solution of such a problem. The resulting temperature dependences of thermodynamic properties include both one-particle effects, connected with VHS, and many-electron Kondo features. Therefore the overall picture is rather complicated. At low temperatures, the Fermi-liquid behavior is restored, except for the case of very small t' . In the latter case, a non-Fermi-liquid behavior takes place which should be studied by more advanced methods.

It would be also of interest to perform similar calculations for the Kondo lattice problem, e.g., in some “mean-field” approximation. A “poor man scaling” approach was applied to this problem in Ref.[38].

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Appendix. Numerical renormalization group approach for the singular density of states

Here we discuss some important details of the numerical renormalization group (NRG) method [2, 40] as applied to our problem of the singular density of states.

Construction of the Wilson chain

Following to Wilson [2] we use a unitary transformation to pass from the operators $c_{\mathbf{k}}$ to the operators f_n . Then the impurity model with a Hamiltonian of type (1) is reduced to a semiinfinite chain (Fig.10) with a Hamiltonian of type:

$$H_{sd} = -J \left[S^+ f_{0\downarrow}^\dagger f_{0\uparrow} + S^- f_{0\uparrow}^\dagger f_{0\downarrow} + S_z \left(f_{0\uparrow}^\dagger f_{0\uparrow} - f_{0\downarrow}^\dagger f_{0\downarrow} \right) \right] + \sum_{\sigma, n=0}^{\infty} \left[\epsilon_n f_{n\sigma}^\dagger f_{n\sigma} + \gamma_n \left(f_{n\sigma}^\dagger f_{n+1\sigma} + f_{n+1\sigma}^\dagger f_{n\sigma} \right) \right], \quad (29)$$

The renormalization group procedure starts from the solution of the isolated-impurity problem (sites “imp” and ϵ_0 in Fig. 10). At the first step, we add a first conducting electronic site ϵ_1 , and construct and diagonalize a Hamiltonian

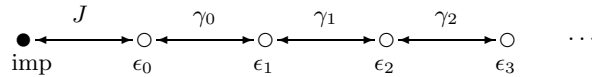


FIG. 10: Representation of the Kondo model in the form of a semiinfinite Wilson chain

matrix on this Hilbert space (with a fourfold higher dimensionality). This procedure is multiply repeated. However, since the dimensionality of Hilbert space grows as 4^N (N is the order number of an iteration), it is impossible to store all the eigenstates during the calculation. Therefore, it is necessary to retain after each iteration only the states with the lowest energies. If we restrict ourselves to a certain maximum number of stored states (determined by the computational possibilities), it is necessary, starting from a certain iteration, to leave of the order of $1/4$ of states at each step.

Unfortunately, direct application of this scheme fails, since the disturbance introduced by the elimination of the high-lying states proves to be too large. Wilson found a method of overcoming this difficulty. This reduces to the artificial introduction of an exponential suppression of matrix elements γ_n , which decreases the coupling between the retained and eliminated states, thereby decreasing the influence of the eliminated states. To this end, Wilson [2] used a logarithmic discretization of the conduction band, i.e., replacement in (1) of an energy range $\epsilon_{\mathbf{k}} \in [\eta D \Lambda^{-m}, \eta D \Lambda^{-m+1}]$,

$\eta = 1, -1$, $m = 1, 2, 3, \dots$ by a single level with an energy $\bar{\varepsilon}_{\eta m}$ equal to the average energy of this interval (D is the half-width of the conduction band, $\Lambda > 1$). This results in a change in the density of states:

$$\rho(\varepsilon) \rightarrow \sum_{\eta, m} \alpha_{\eta m}^2 \delta(\varepsilon - \bar{\varepsilon}_{\eta m}) , \quad (30)$$

where

$$\alpha_{\eta m}^2 = \eta \int_{\eta D \Lambda^{-m}}^{\eta D \Lambda^{-m+1}} \rho(\varepsilon) d\varepsilon .$$

As a result, the jumps will have the required decay, $\gamma_n \propto \Lambda^{-n/2}$; for a flat band, Wilson obtained analytically

$$\gamma_n = \frac{D(1 + \Lambda^{-1})(1 - \Lambda^{-n-1})}{2\sqrt{1 - \Lambda^{-2n-1}}\sqrt{1 - \Lambda^{-2n-3}}} \Lambda^{-n/2} , \epsilon_n = 0 . \quad (31)$$

In more complicated situations, the construction of the Wilson chain must be performed numerically. Usually (see, e.g., Ref.[41]) this is performed in spirit of the initial work [2], by numerical reproducing Wilson's analytical flat-band procedure for an arbitrary density of states. However, there exists another way which yields equivalent results, but seems to be more natural. To bring the Hamiltonian matrix

$$H_\sigma = \sum_{\eta, m} \bar{\varepsilon}_{\eta m} c_{\eta m, \sigma}^\dagger c_{\eta m, \sigma} \quad (32)$$

to the tridiagonal form, one can use the Lanczos tridiagonalization algorithm [42] which is just adapted namely for this problem. For the model (1) this method was described in Ref.[4] where a Wilson chain for non-discretized semielliptic density of states was also analytically constructed. We perform this procedure numerically for an arbitrary logarithmically discretized density of states. Starting from the vector $|0\rangle = f_{0\sigma}^\dagger |\text{vac}\rangle$ (where $f_{0\sigma}^\dagger = \sum_{\eta, m} \alpha_{\eta m} c_{\eta m, \sigma}^\dagger$) we generate a new basis $|0\rangle, |1\rangle, |2\rangle, \dots$ for the conduction electron states by Schmidt orthogonalization:

$$\begin{aligned} |1\rangle &= \frac{1}{\gamma_0} (H_\sigma |0\rangle - |0\rangle \langle 0| H_\sigma |0\rangle) , \\ |2\rangle &= \frac{1}{\gamma_1} (H_\sigma |1\rangle - |1\rangle \langle 1| H_\sigma |1\rangle - |0\rangle \langle 0| H_\sigma |1\rangle) , \\ |n+1\rangle &= \frac{1}{\gamma_n} (H_\sigma |n\rangle - |n\rangle \langle n| H_\sigma |n\rangle - |n-1\rangle \langle n-1| H_\sigma |n\rangle) , \end{aligned} \quad (33)$$

where each γ_n is chosen to normalize $|n+1\rangle$. One can see that $\langle n'| H_\sigma |n\rangle = 0$ for $n' = 0, 1, 2, \dots, n-2$. This means that H_σ is tridiagonal in the new basis. The off-diagonal elements are $\langle n+1| H_\sigma |n\rangle = \gamma_n$. Defining $\epsilon_n \equiv \langle n| H_\sigma |n\rangle$ we consecutively obtain the coefficients γ_n and ϵ_n for (29).

Calculation of thermodynamical averages

In our calculations we put $\Lambda = 1.5$ and store 10^4 states per iteration.

Diagonalizing the Hamiltonian (29) for a given chain length N yields a set of eigenvalues. As indicated in Ref.[2], because of retaining only part of the energy spectrum at the N -th step of the NRG procedure, thermodynamic averages should be calculated at a temperature that depends on Λ : $T_N = \Lambda^{-N/2} T_0$, where the starting temperature T_0 is chosen more or less arbitrarily. However, it should be neither too large (then the contributions of abandoned high-energy states becomes important), nor too small (then the discreteness of the energy spectrum becomes appreciable).

The total entropy and specific heat read [40]

$$\begin{aligned} \mathcal{S}_{\text{tot}} &= \langle H \rangle_{\text{tot}} / T + \ln Z_{\text{tot}} , \\ C_{\text{tot}} &= [\langle H^2 \rangle_{\text{tot}} - \langle H \rangle_{\text{tot}}^2] / T^2 , \end{aligned} \quad (34)$$

where Z is partition function. Since the total spin commutes with the Hamiltonian H , each eigenvalue is characterized by a well-defined spin projection $S_{z, \text{tot}}$, therefore the quantities like $\langle S_z^2 \rangle_{\text{tot}}$ can be calculated straightforwardly. On differentiating $\langle S_z \rangle_{\text{tot}}$ with respect to magnetic field one obtains [2]

$$T \chi_{\text{tot}}(T) = [\langle S_z^2 \rangle_{\text{tot}} - \langle S_z \rangle_{\text{tot}}^2] , \quad (35)$$

$T\chi_{\text{band}}(T)$, $\mathcal{S}_{\text{band}}$ and C_{band} are calculated in a similar way, and the corresponding impurity contributions are obtained by subtracting them from (34)-(35).

Because of finite length of the chain, the thermodynamic quantities like $T_N\chi_{\text{imp}}(T_N)$ and $C_{\text{imp}}(T_N)$ demonstrate even-odd oscillations depending on T_N which have nearly constant amplitude. Therefore the amplitude of the oscillations in $\chi(T)$ and $C(T)/T = \gamma(T)$ increases strongly with lowering T .

To suppress the oscillations in $\chi(T)$, we used smoothing according to Euler [43]. If there is a certain oscillating sequence A_n , we introduce a new sequence $A_n^{(1)}$ whose members are equal to averages of the adjacent members of the initial sequence: $A_n^{(1)} = (A_n + A_{n+1})/2$. If necessary, the procedure is repeated: $A_n^{(2)} = (A_n^{(1)} + A_{n+1}^{(1)})/2$. In particular, this was made in the calculation of χ_{imp} . By designating $\chi_N \equiv \chi_{\text{imp}}(T_N)$, we obtain

$$\begin{aligned}\chi^{(1)}(\sqrt{T_N T_{N+1}}) &= \frac{1}{2}\chi_N + \frac{1}{2}\chi_{N+1} \\ \chi^{(2)}(T_N) &= \frac{1}{4}\chi_{N-1} + \frac{1}{2}\chi_N + \frac{1}{4}\chi_{N+1} \\ \chi^{(3)}(\sqrt{T_N T_{N+1}}) &= \frac{1}{8}\chi_{N-1} + \frac{3}{8}\chi_N + \frac{3}{8}\chi_{N+1} + \frac{1}{8}\chi_{N+2}\end{aligned}\tag{36}$$

A similar problem which occurs at calculating the slope of specific heat γ_{imp} is solved by the same way. The method was tested for the flat-band case to obtain the values $R = 2.008, 2.016$ and $w = 0.416, 0.417$ for $J = -0.1, -0.2$ respectively (cf. Table 1). Our method differs from [2] by that we calculate χ and γ directly rather than by constructing an effective Hamiltonian explicitly near the fixed point $J = -\infty$. Although resulting in a slight decrease of accuracy, such an approach can be applied more widely, in particular to obtain a NFL behavior (see Figs.4-6).

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